Supplementary Information for Identification of key interactions between SARS-CoV-2 Main Protease and inhibitor drug candidates

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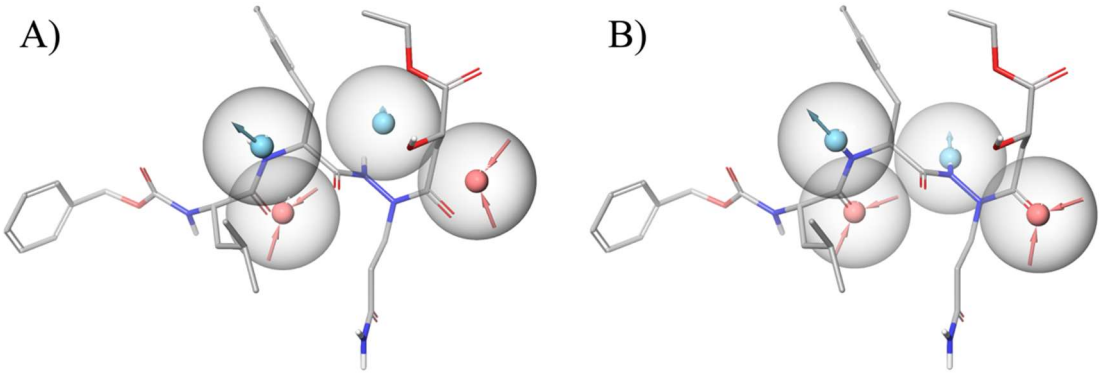

Figure S1. Pharmacophore model candidates constructed by SARS-CoV M^{pro}-inhibitor complex structure. Four features of inhibitors that bind to SARS-CoV M^{pro} were extracted. Blue spheres indicate H-bond donor (HBD), and red spheres indicates H-bond acceptor (HBA). Pharmacophore models were aligned with 2A5I ligand (Grey stick model). A: Used model (screen score: 5.34). B: Unused model (screen score: 5.07).

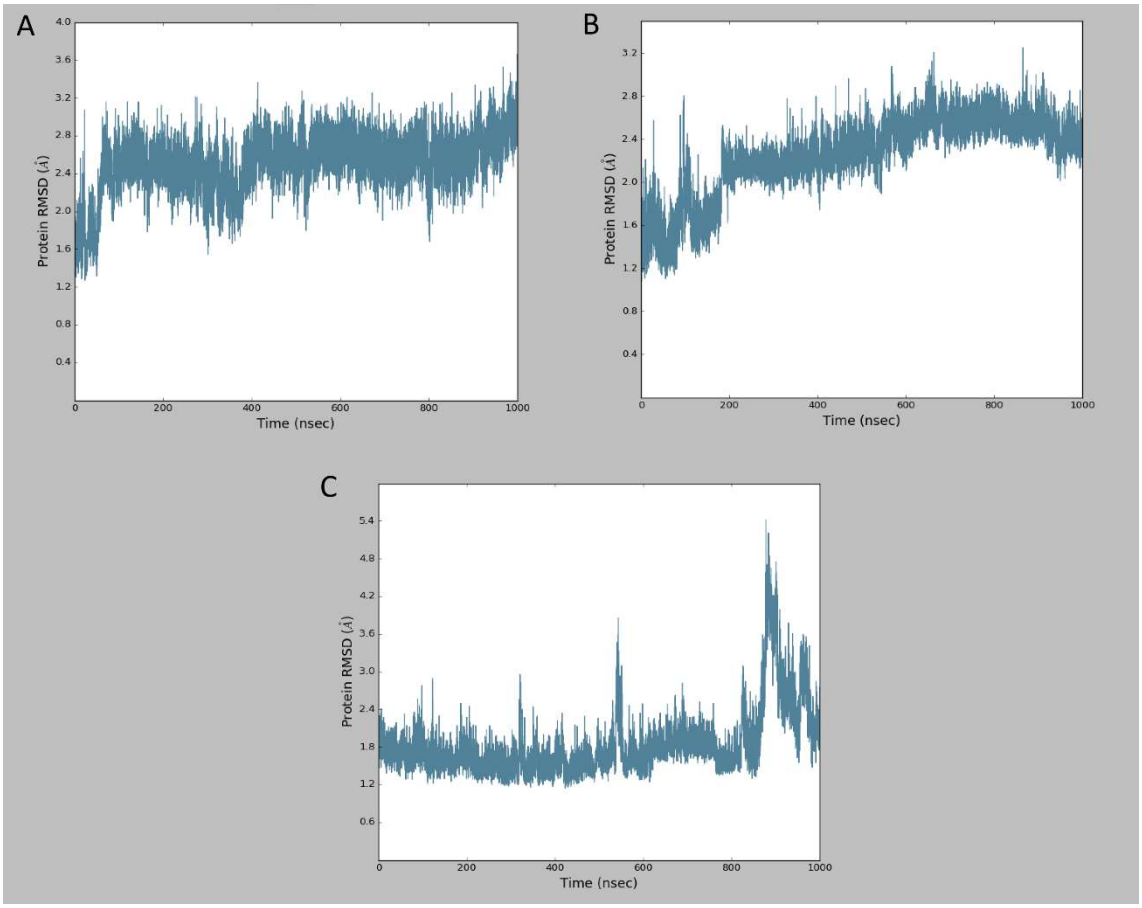

Figure S2. Root mean square deviations of SARS-nCoV-2 M^{pro} C_α atoms in the MD simulations. A: 2A5I ligand complex model, B: 2OP9 ligand complex model, C: Indinavir complex model

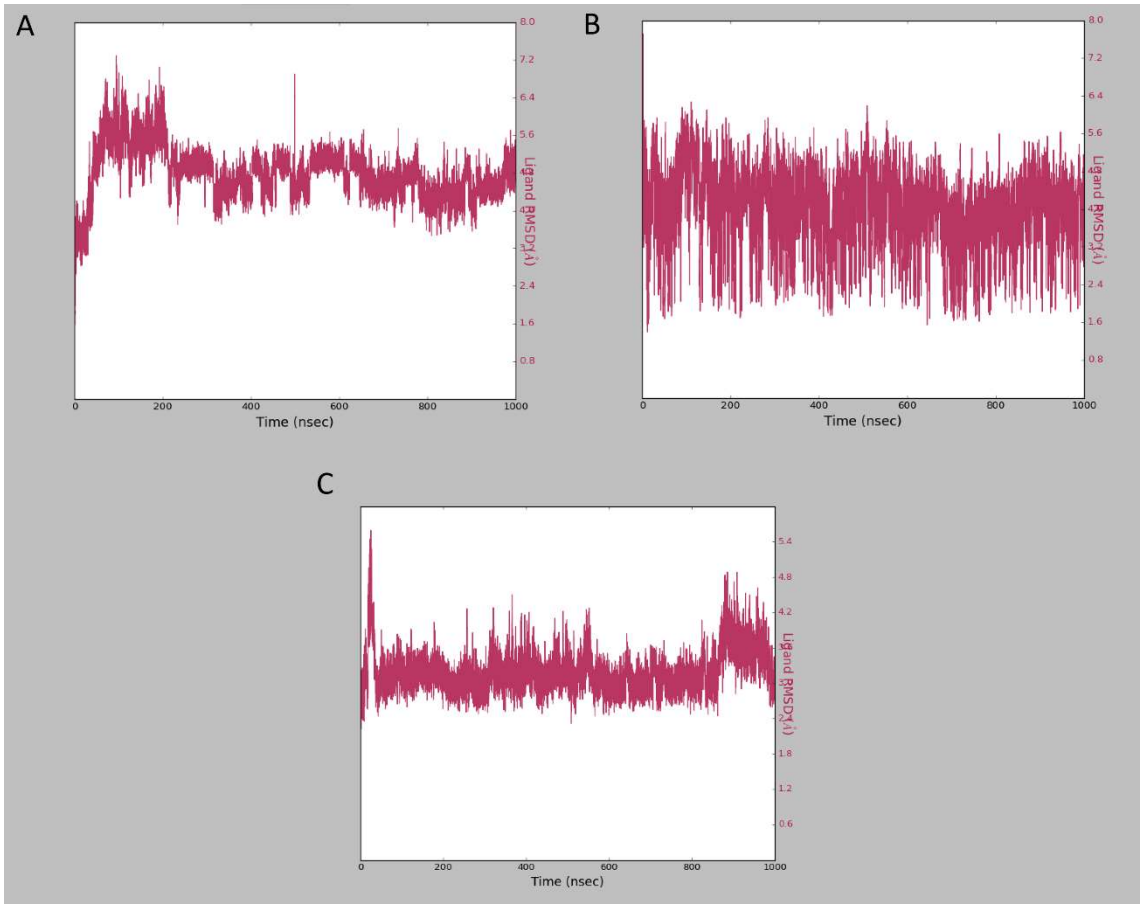

Figure S3. Root mean square deviations of ligand atoms in the MD simulations. A: 2A5I ligand, B: 2OP9 ligand, C: Indinavir

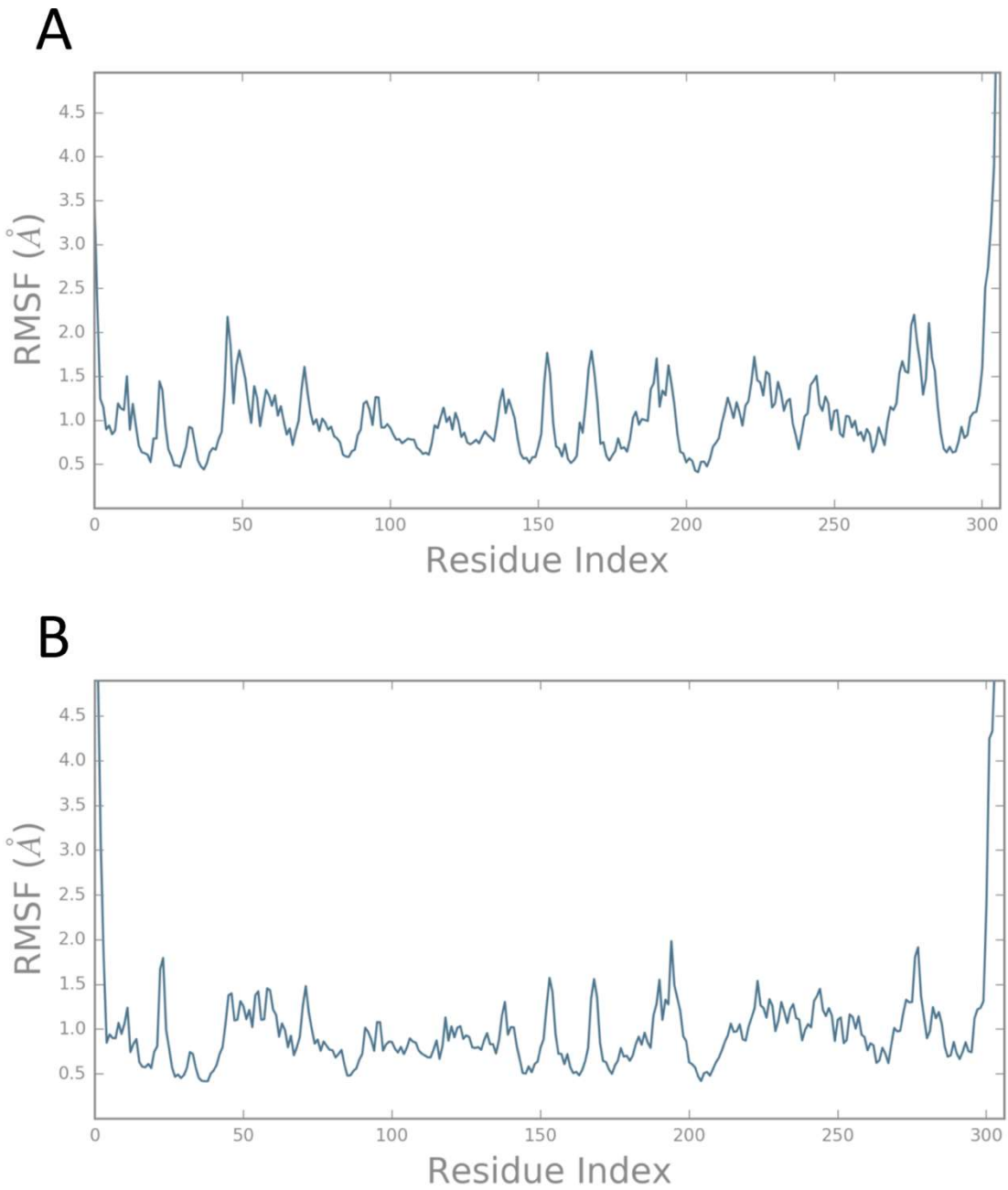

Figure S4. Root-mean-square fluctuation of amino acid residue in the MD simulations. A: 2A5I ligand, B: 2OP9 ligand

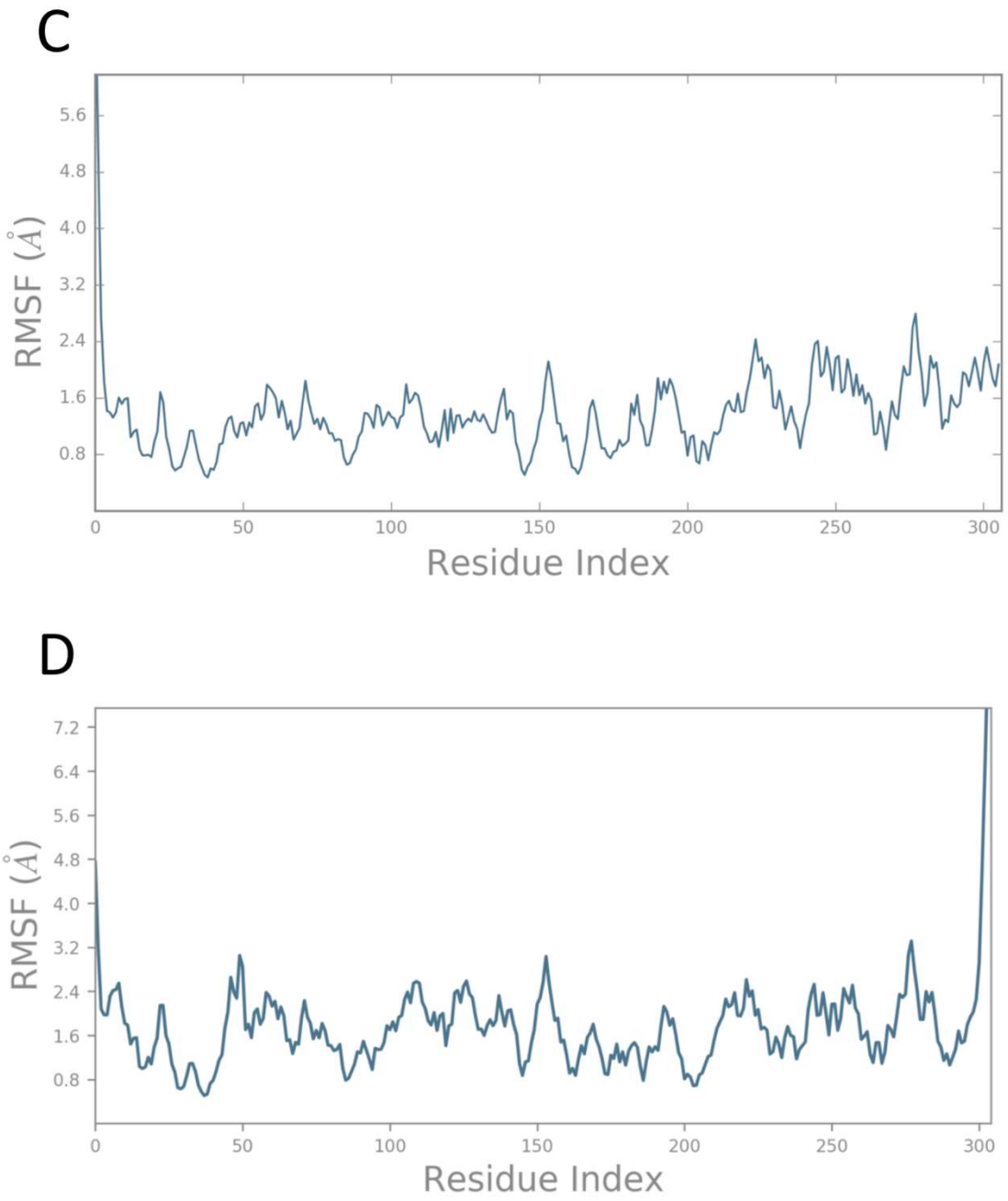

Figure S4. Continued. C: Indinavir, D: 6LU7 apo form

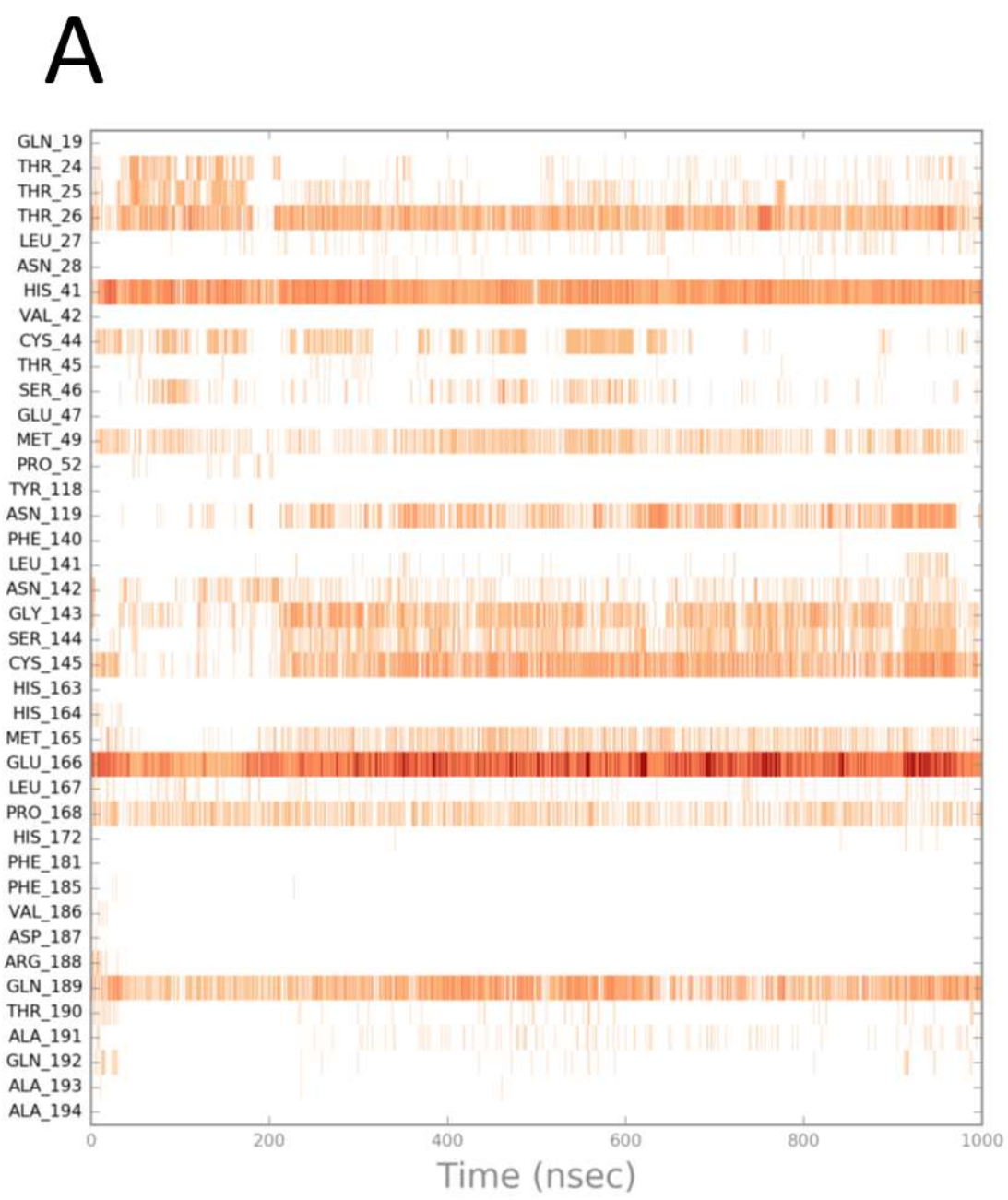

Figure S5. Timeline representation of the interactions and contacts (H-bonds, Hydrophobic, Ionic, Water bridges). This figure shows which residues interact with the ligand in each trajectory frame. Some residues make more than one specific contact with the ligand, which is represented by a darker shade of orange. A: 2AI5 Ligand.

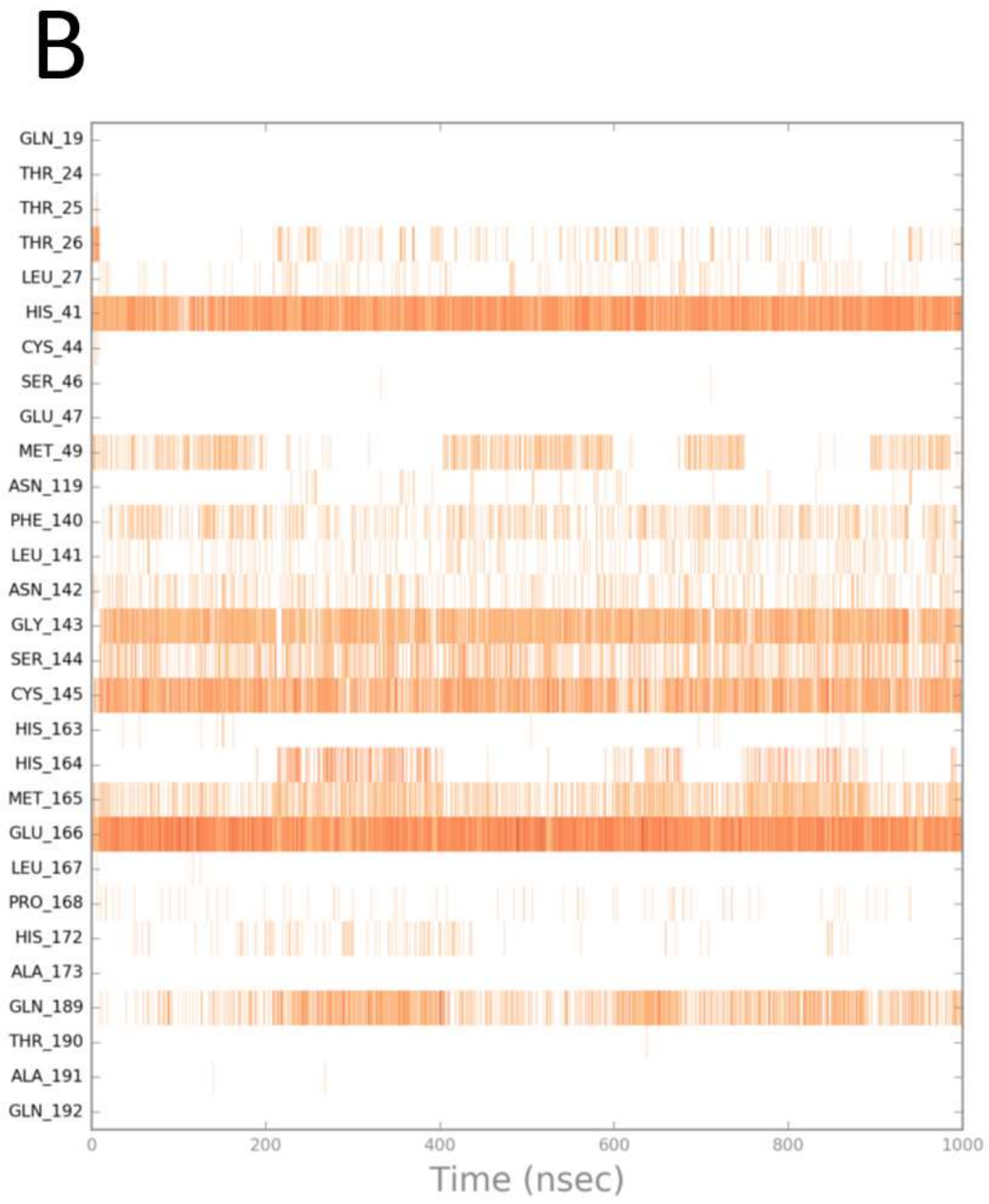

Figure S5. Continued. B: 2OP9 Ligand.

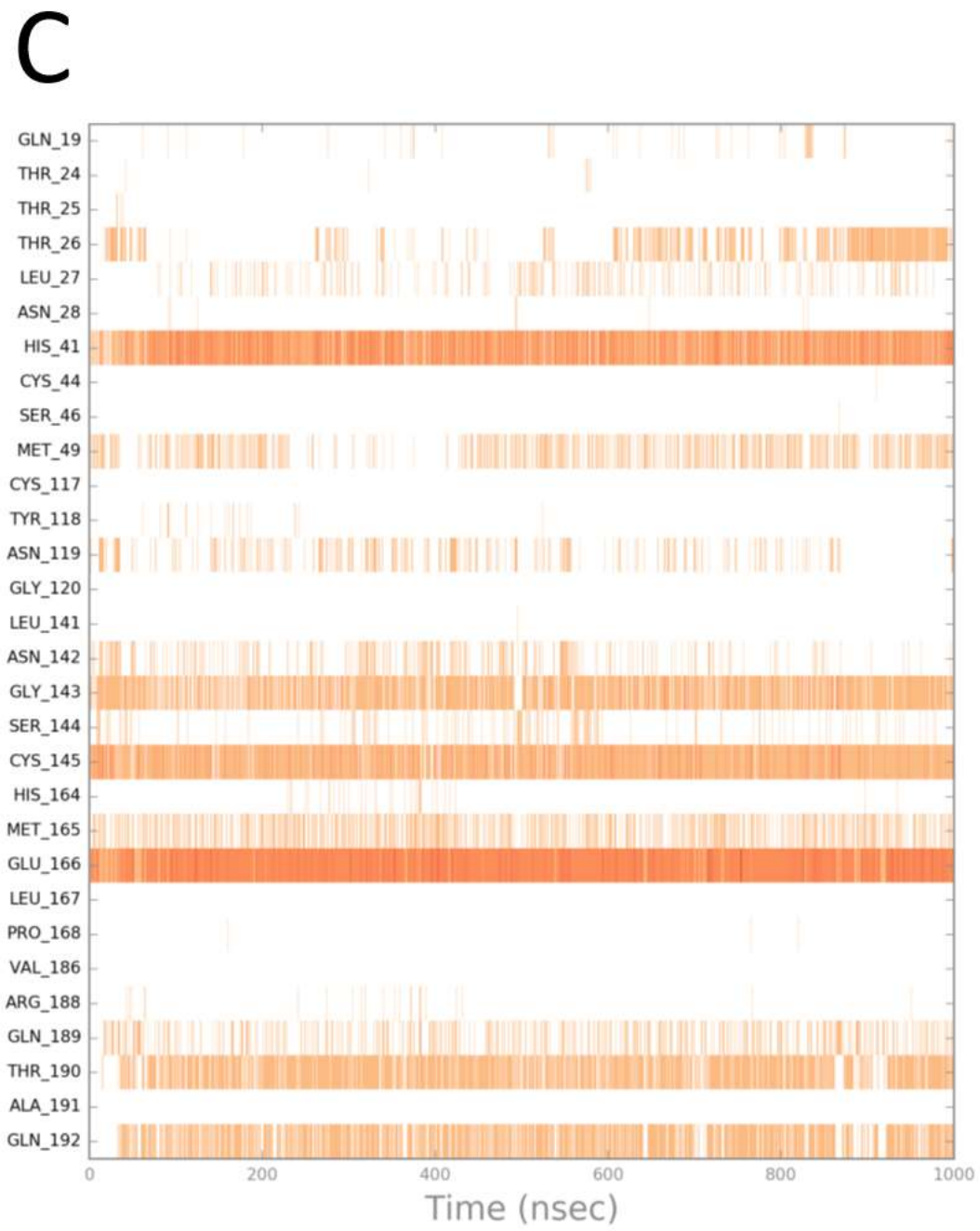

Figure S5. Continued. C: Indinavir.